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**THE LONGWAVE SILICON CHIP - INTEGRATED PLASMA-
PHOTONICS IN GROUP IV AND III-V SEMICONDUCTORS**

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Final Report**

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14. ABSTRACT This Report presents results obtained on a three-year basic research project intended to advance the science and technology of nano-photonics, electro-optics, and nano-plasmonics integrated on a silicon opto-electronic chip that operates in the 1.3 to 5.0 micron wavelength range. Original contributions were made in group IV photonics for mid-infrared applications; SiGeSn heterostructure photonics; group IV plasmonics, Franz-Keldysh modulation in GeSn; electro-optical logic; reconfigurable optoelectronics; free carrier electro-modulation; band-to-band GeSn MQW laser diodes; GeSn photodiodes and LEDs; SiGe third-order nonlinear optics. Many additional topics were investigated.					
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**The Longwave Silicon Chip: Integrated Plasmo-Photonics
in Group IV and III-V Semiconductors**

AFOSR grant FA9550-10-1-0417

Principal Investigators: Greg Sun and Richard Soref

The University of Massachusetts at Boston

Physics Department and the Engineering Program

Executive Summary: This Final Report presents results obtained on a three-year basic research project intended to advance the science and technology of nano-photonics, electro-optics, and nano-plasmonics integrated on a silicon opto-electronic chip that operates in the 1.3 to 5.0 micron wavelength range. Invention, discovery, physics insight, numerical modeling, simulation, device design and device optimization were the approaches taken on this project. Original, leading-edge contributions were made in the areas of: group IV photonics for mid-infrared applications; SiGeSn heterostructure photonics; group IV plasmonics with silicides, germanicides, doped Si, Ge or GeSn; Franz-Keldysh modulation in GeSn; electro-optical logic; reconfigurable optoelectronics; free carrier electro-modulation over the mid infrared; band-to-band GeSn MQW laser diodes; GeSn photodiodes; third-order nonlinear optics in Si, SiGe and Ge; second-order nonlinear optics in strained Si; GeSn LEDs; group IV intersubband lasers; metamaterials; perfect infrared absorbers; ultralow-energy carrier-depletion modulation in resonant Si nano-beams and MOS microdonuts; gap-plasmon waveguides; nano-spasers; and metal nano-particle arrays for plasmonic enhancement of detection and luminescence.

1. Objectives of the Project: The main goal of this 3-year basic research project was to advance the science and technology of silicon-based nanophotonics and nanoplasmonics for telecom/datacom and the newer mid-infrared applications such as chem-bio-physico sensing, medical/health uses, and environmental monitoring. All results on this project are intended to be compatible with Si opto-electronic integrated “circuit” chips that are manufactured in a modern CMOS foundry. The science goal includes investigation of the emerging GeSn and SiGeSn heterostructure material systems that provide monolithic Group IV integration on the OEIC, although III-V semiconductor hybrid-integration-on-Si is another aspect of this project. An added objective is the invention of new and/or higher performance electro-optical devices including modulators, switches, lasers, light-emitting diodes, photodetectors, infrared amplifiers and nonlinear optical devices. In terms of wavelength, the telecom devices investigated operate in the new 2 μm band or in 1.31-1.55 μm . The “beyond telecom” devices cover 2 to 5 μm .

2. Approaches taken on this Project: Waveguided and free-space structures were studied, with a strong emphasis on waveguided devices. For photonic devices, the diffraction limit of classical optics sets a lower limit on the useable device cross-section dimensions at $\sim \lambda/2n$; whereas the plasmonic devices can go well below the diffraction limit in their footprint and in their cross-section dimensions. Those dimensions can be deep subwavelength. Plasmonics and photonics are compatible in the sense that the electromagnetic propagating mode in a photonic device can couple to the SPP mode in a plasmonic device, and vice versa. The two types of devices can share some of the same construction materials; for example, in the Si-based Group IV photonics case, a Si or Ge or GeSn dielectric core can be “shared” with an SPP waveguide in which localized silicide or germanicide “conductors” are introduced to give local plasmonic confinement.

Therefore, guided-wave photonics can be closely integrated with guided-wave plasmonics to make synergistic “plasmo-photonic” structures that, however, bring a tradeoff of higher propagation losses in the SPP region--indicating that the plasmonic structures will be mainly compact “discrete” devices that are situated within an extended or distributed photonic network system. In the plasma-photonic network, value is added by making the plasmonic devices active, for example, by creating a voltage-controlled MOS charge accumulation layer in the device. Then, because of its ultracompact size, the device will offer 100 Gb/s switching speeds with switching energies below 1 fJ/bit.

The approaches taken on this project combine theory and experiment with a strong emphasis upon theory performed at UMB. Approaches include physics discovery, vision, invention, device design, simulation, optimization and numerical modeling to predict and enable new and/or higher performance. Experiments in support of this grant were performed at the Universities listed in Section 3 below. Section 3 specifies the outstanding expert assistance given to the PIs on this program.

3. Scientific collaborators on this project: A complete list of results is given below in Section 4. The list of co-authors in Section 4 is very long and here we wish to single out the primary collaborators who are senior scientific colleagues at other universities and at Air Force laboratories. The PIs were fortunate to have collaborators *who provided experiments and/or theory work for this project at no cost to AFSOR:*

The first group of collaborators contributed work on theory and experiment: Henry H. Cheng, NTU; Robert Peale, UCF; Qianfan Xu, Rice Univ; Weidong Zhou, UT Arlington; Wei Jiang, Rutgers; Jack Ma, Univ Wisconsin; Goran Masanovich, Univ Southampton; Fisher Yu, Univ Arkansas; and Volker Sorger, GWU. A second group of collaborators gave expert collaboration on theory: Walter Buchwald, UMass Boston; Justin Cleary, AFRL; Joshua Hendrickson, AFRL; Jacob Khurgin, Johns Hopkins; Zoran Ikonc, Univ Leeds; James Kolodzey, Univ Delaware, Bahram Jalali, UCLA; Ivan Avrutsky, Wayne State Univ; Milos Nedeljkovic, Univ Southampton; Junpeng Guo, Univ Alabama Huntsville; Sang-Yeon Cho, New Mexico State Univ; and Jaeyoun Kim, Iowa State Univ.

4. Summary of Results. The accomplishments of this project are summarized by listing the book chapters, peer-reviewed journal publications, invited lectures, invited plenary talks, invited conference papers, contributed conference papers, editorial assignments, and conference organizer contributions.

List of All Results on this AFOSR Grant

(in reverse chronological order from 31 Aug 2013 back to 31 Aug 2010)

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5. Highlights of Results Listed Above: These results are wide-ranging, extensive and voluminous. The results show innovation/discovery and detailed study/fulfillment of the topics and milestones set forth in the original 2010 grant proposal. We believe that AFOSR and the S&T community shall be able to transition these results to advanced technology. These contributions are original and several are “world firsts.” Some highlights are: the second-order nonlinear response of strained silicon waveguides, the gap plasmon mode in silicon based hybrid waveguides, broadband metamaterials, reconfigurable integrated optoelectronics, electro-optical logic in silicon, silicides for group IV plasmonics, reviews of third-order nonlinear optical coefficients in Si, SiGe and Ge, nano-spaser design, the plasmonics of n-GeSn and n-Ge, Franz-Keldysh electro-absorption modulation in GeSn, design of GeSn/SiGeSn multi-quantum-well laser diodes, first-principles band theory of all SiGeSn alloys, Fano nano-membrane devices, ultralow-energy MOS microdonut and PN nanobeam depletion modulators, perfect absorbers for LWIR, and free carrier electro-modulation of Si over 1 to 14 micron wavelengths. An important series of surface plasmon papers focused on nano-spasers, and on metal nano-particle enhancements of detection, Raman scattering, fluorescence and photoluminescence. Two results are perhaps the most noteworthy. The first is the vision of migrating Group IV photonics into the mid infrared. This was detailed in the Nature Photonics article and in the Plenary talk (with a 15-page manuscript published in the Proceedings) presented at the 2013 SPIE Photonics West Conferences. The talk had an audience of 450 and received 350 views on YouTube. The second is the invited talk on SiGeSn heterostructure photonics (with manuscript printed in the Philosophical Transactions) presented at the Royal Society of London.

6. Selected Illustrations of the Results In this section, we present Figures that were reproduced from our peer-reviewed publications cited above. These illustrations represent *a small sample* of the progress presented in Section 4.

Illustration 1: Electro-optical logic in SOI

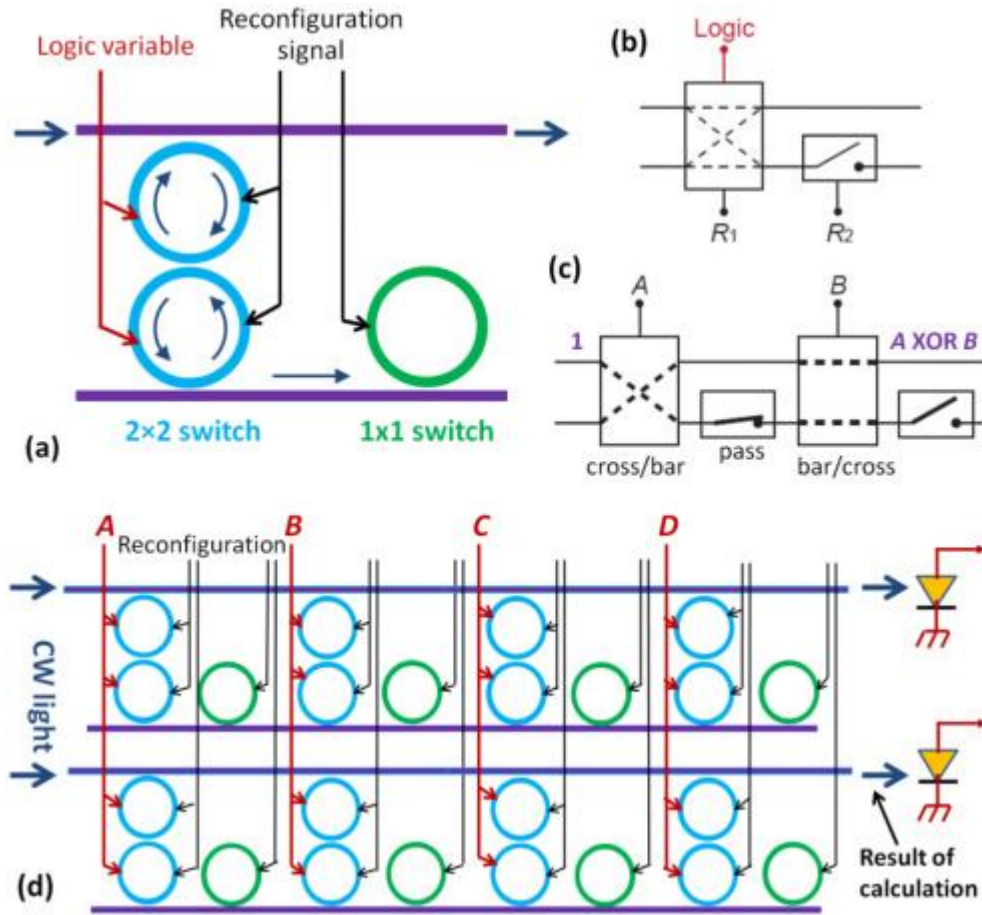


Figure 1. Electro-optical logic cellular array proposed by UMB for group IV photonics.

We present a reconfigurable optical directed logic architecture that offers several significant improvements over the original directed logic presented by Hardy and Shamir. Specific embodiments of on-chip, waveguided, large-scale-integrated, cellular optical directed logic fabrics are proposed and analyzed. Five important logic functions are presented as examples to show that the same switch fabric can be reconfigured to perform different logic functions.

Illustration 2: MOS depletion-type modulator and switch

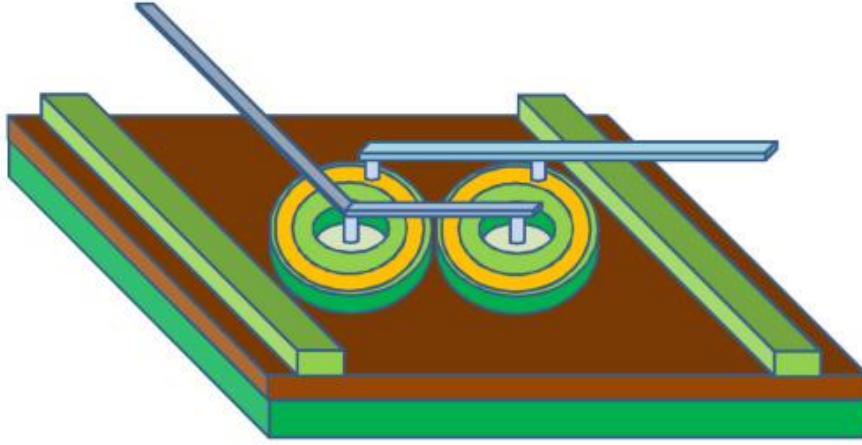


Figure 2. Electro-optical MOS 2 x 2 switch proposed by UMB for SOI photonics.

Electrical, optical and electro-optical simulations are presented for a waveguided, resonant, bus-coupled, *p*-doped Si micro-donut MOS depletion modulator operating at the 1.55 μm wavelength. To minimize the switching voltage and energy, a high-K dielectric film of HfO_2 or ZrO_2 is chosen as the gate dielectric, while a narrow ring-shaped layer of *p*-doped poly-silicon is selected for the gate electrode, rather than metal, to minimize plasmonic loss loading of the fundamental TE mode. In a 6- μm -diam high-Q resonator, an infrared intensity extinction ratio of 6 dB is predicted for a modulation voltage of 2 V and a switching energy of 4 fJ/bit. A speed-of-response around 1 ps is anticipated. For a modulator scaled to operate at 1.3 μm , the estimated switching energy is 2.5 fJ/bit.

Illustration 3: GeSn/GeSiSn laser diode on silicon

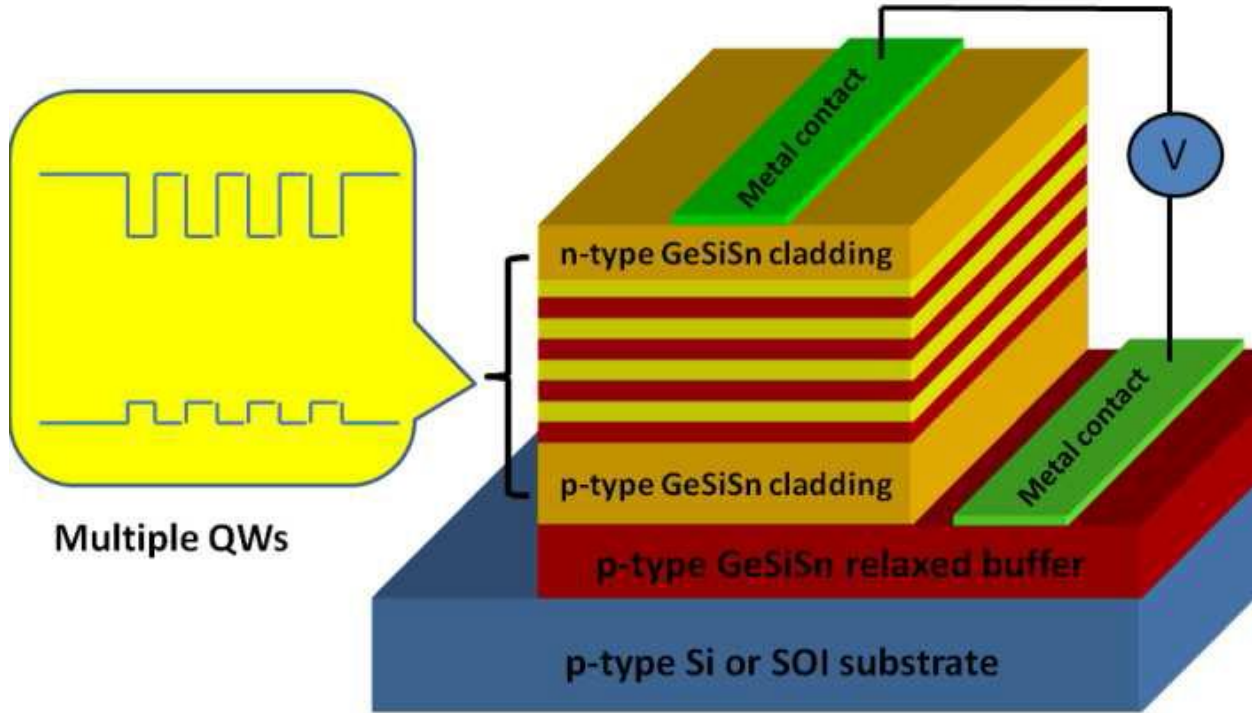


Figure 3. GeSn/SiGeSn multi-quantum-well laser diode designed by UMB.

This paper presents modeling and simulation of a silicon-based group IV semiconductor injection laser diode in which the active region has a multiple quantum well structure formed with $\text{Ge}_{0.9}\text{Sn}_{0.1}$ quantum wells separated by $\text{Ge}_{0.75}\text{Si}_{0.1}\text{Sn}_{0.15}$ barriers. These alloy compositions were chosen to satisfy three conditions simultaneously: a direct band gap for $\text{Ge}_{0.9}\text{Sn}_{0.1}$, type-I band alignment between $\text{Ge}_{0.9}\text{Sn}_{0.1}$ and $\text{Ge}_{0.75}\text{Si}_{0.1}\text{Sn}_{0.15}$, and a lattice match between wells and barriers. This match ensures that the entire structure can be grown strain free upon a relaxed $\text{Ge}_{0.75}\text{Si}_{0.1}\text{Sn}_{0.15}$ buffer on a silicon substrate – a CMOS compatible process. Detailed analysis is performed for the type I band offsets, carrier lifetime, optical confinement, and modal gain. The carrier lifetime is found to be dominated by the spontaneous radiative process rather than the Auger process. The modal gain has a rather sensitive dependence on the number of quantum wells in the active region. The proposed laser is predicted to operate at $2.3\ \mu\text{m}$ in the mid infrared at room temperature.

Illustration 4: Bandgap theory of unstrained SiGeSn alloy

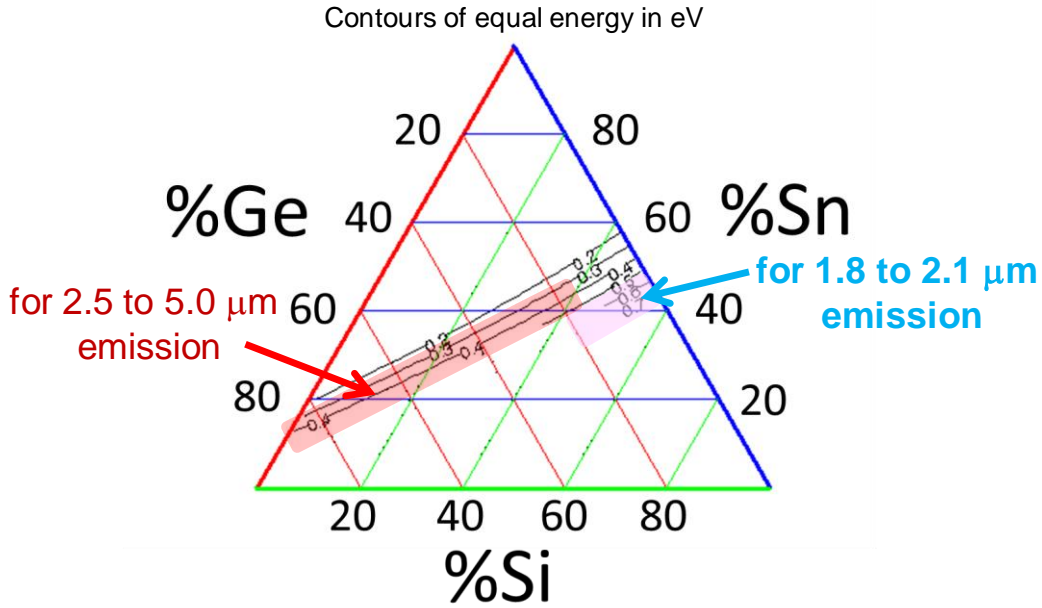


Figure 4. Direct bandgap of various SiGeSn alloy compositions predicted by UMB for lasing and other group IV opto-electronic applications.

Using empirical pseudopotential theory, the direct (Γ) and indirect bandgaps (L and X) of unstrained crystalline $\text{Si}_x\text{Ge}_{1-x-y}\text{Sn}_y$ have been calculated over the entire xy composition range. The results are presented as energy-contour maps on ternary diagrams along with a ternary plot of the predicted lattice parameters. A group of 0.2 to 0.6 eV direct-gap SiGeSn materials is found for a variety of mid-infrared photonic applications. A set of “slightly indirect” SiGeSn alloys having a direct gap at 0.8 eV (but with a smaller L- Γ separation than in Ge) have been identified. These materials will function like Ge in various telecom photonic devices. Hetero-layered SiGeSn structures are described for infrared light emitters, amplifiers, photodetectors, and modulators (free carrier or Franz-Keldysh). We have examined in detail the optimized design space for mid-infrared SiGeSn-based multiple-quantum-well laser diodes, amplifiers, photodetectors, and quantum-confined Stark effect modulators.

Illustration 5: Plasmonics in heavily doped GeSn

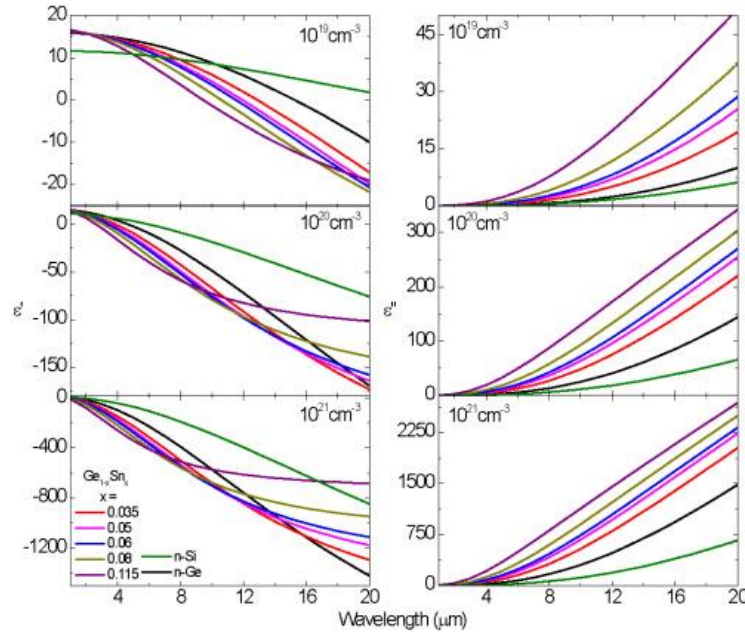


Figure 5. Theory developed by UMB showing the MWIR and LWIR wavelength regions of negative real permittivity (left) and imaginary permittivity (right) for heavily n-doped GeSn, Ge and Si.

Heavily doped n-type Ge and GeSn are investigated as plasmonic conductors for integration with undoped dielectrics of Si, SiGe, Ge, and GeSn in order to create a foundry-based group IV plasmonics technology. N-type $\text{Ge}_{1-x}\text{Sn}_x$ with compositions of $0 \leq x \leq 0.115$ are investigated utilizing effective-mass theory and Drude considerations. The plasma wavelengths, relaxation times, and complex permittivities are determined as functions of the free carrier concentration over the range of 10^{19} to 10^{21} cm^{-3} . Basic plasmonic properties such as propagation loss and mode height are calculated and example numerical simulations are shown of a dielectric-conductor-dielectric ribbon waveguide structure are shown. Practical operation in the 2 to 20 μm wavelength range is predicted.

Illustration 6: Fano membrane LWIR reflectors in silicon

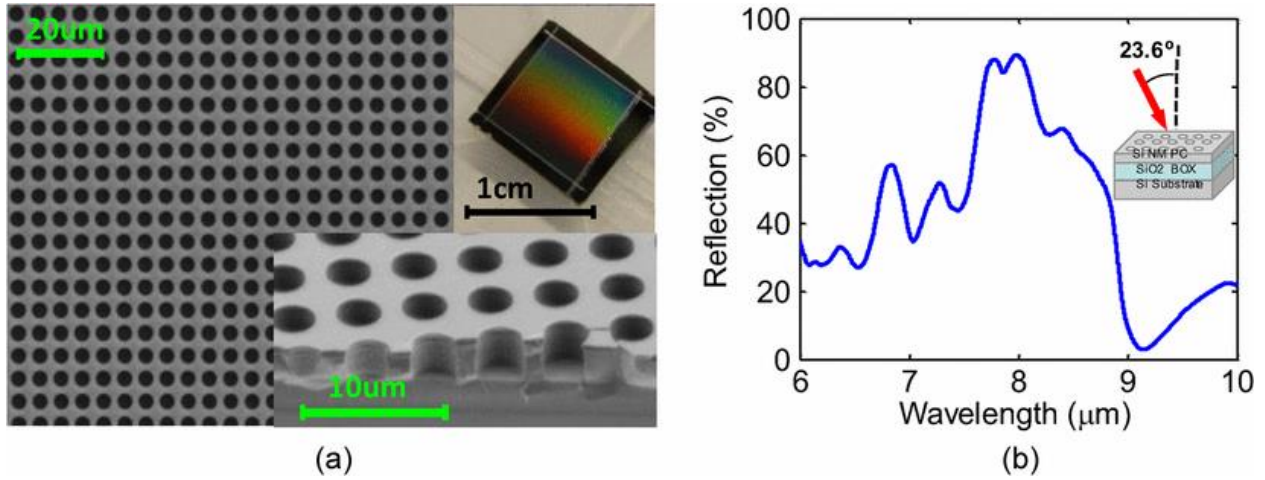


Figure 6. Silicon photonic crystal Fano nano-membrane for LWIR reflection.

The authors report here single layer ultra-compact Si MRs at mid-infrared and far-infrared bands, based on suspended air-clad structure. High performance reflectors were designed for surface- normal incidence with center operation wavelengths of 1.5 μm, ~ 8 μm, and 75 μm, respectively. Large area patterned membrane reflectors were also fabricated and transferred onto glass substrates based on PDMS stamp assisted membrane transfer process. Close to 100% reflection was obtained at ~76 μm, with a single layer Si membrane thickness of 18 μm.

Illustration 7: Free-carrier response of Si at MWIR and LWIR

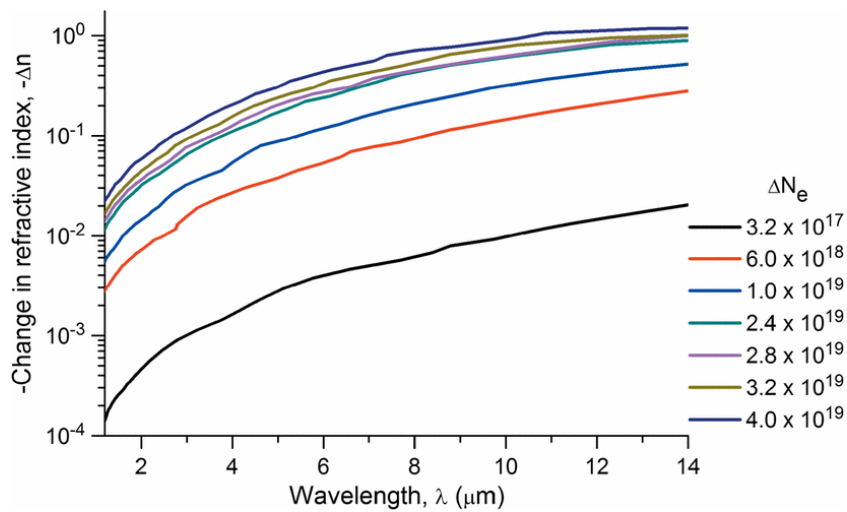


Figure 7. Predicted-by-UMB change in the real index of Silicon over the MWIR and LWIR wavelength range; an index shift produced by the change in free electron concentration.

We present relationships for the free-carrier-induced electrorefraction and electroabsorption in crystalline silicon over the 1-14- μm wavelength range. Electroabsorption modulation is calculated from impurity-doping spectra taken from the literature, and a Kramers-Kronig analysis of these spectra is used to predict electrorefraction modulation. More recent experimental results for terahertz absorption of silicon are also used to improve the commonly used 1.3- and 1.55- μm equations. We examine the wavelength dependence of electrorefraction and electroabsorption, finding that the predictions suggest longer wave modulator designs will, in many cases, be different from those used in the telecom range.

Illustration 8: The case for using gap plasmon-polaritons in second-order optical nonlinear processes

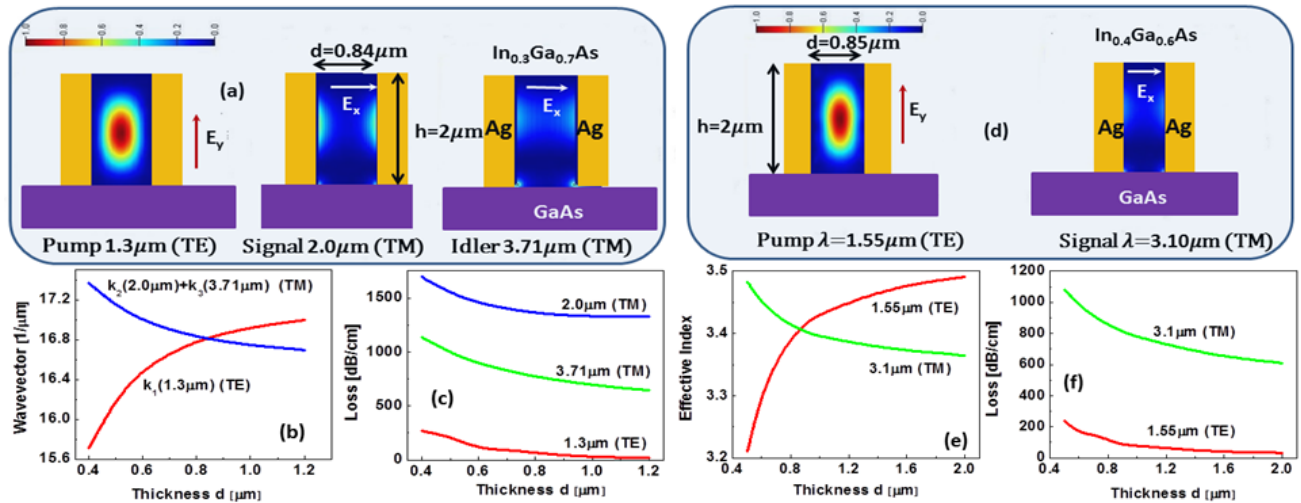


Figure 8. (a) Power densities of TE pump and TM signal and idler waves in the MIM waveguide designed for DFG at 3710 nm, (b) propagation constants, (c) loss of these modes as a function of waveguide width d , (d) power densities of TE pump and TM signal waves in the MIM waveguide designed for degenerate OPG at 3100 nm, (e) effective indices, and (f) loss of these modes as a function of waveguide width d .

In this work, we show that using metal-insulator-metal (MIM) waveguides to carry out various second-order nonlinear optical processes not only provides highly desired tight optical confinement but also facilitates the phase-matching due to their inherently large anisotropy. This fact allows one to take advantage of otherwise inaccessible large nonlinear susceptibilities of the cubic zinc blende

semiconductors. Our efficiency estimates show that since only the longer wavelength infra-red radiation propagates in the surface-plasmon-polariton (SPP) mode, the losses in the metal, while significant, do not preclude development of highly compact nonlinear optical devices on this integration-friendly semiconductor platform.

Illustration 9: Origin of giant difference between fluorescence, resonance and non-resonance Raman scattering enhancement by surface plasmons

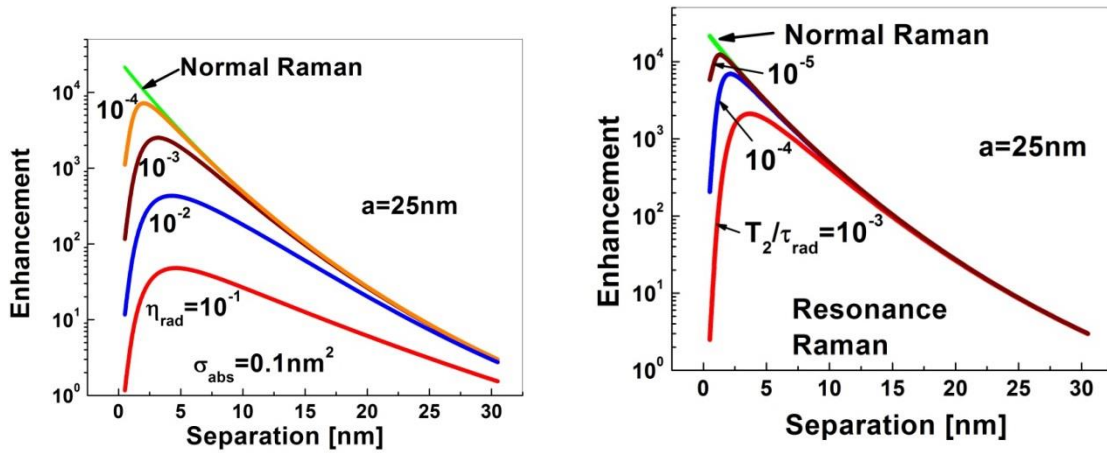


Figure 9. Comparison between Raman and fluorescence enhancement for a range of molecules with $\sigma_{abs} = 0.1 \text{ nm}^2$ and $10^{-4} \leq \eta_{rad} \leq 10^{-1}$ for an Au sphere of radius $a = 25 \text{ nm}$. Quenching of resonance Raman for a range of molecules with T_2 / τ_{rad} ratio varying from 10^{-5} to 10^{-3} near an Au sphere of radius $a = 25 \text{ nm}$, compared with normal Raman enhancement.

In this work, we compare plasmonic enhancement for fluorescence, resonance and off-resonance Raman spectroscopy which are all precise and versatile techniques for indentifying small quantities of chemical and biological substances. One way to improve the sensitivity and specificity of these measurement techniques is to use enhancement of optical fields in the vicinity of metal nanoparticles. The degree of enhancement, however, is drastically different as Raman enhancement of 10 orders of magnitude or more has been consistently measured in experiment, while the enhancement of the seemingly similar process of fluorescence is typically far more modest. While resonance Raman scattering has the advantages of higher sensitivity and specificity when compared with the ordinary, non-resonant Raman process, its plasmon enhancement is far less spectacular. In fact, both fluorescence and resonance Raman measurements are subject to quenching when the molecule is

placed too close to the metal surface, such an effect, however, is completely absent from the normal non-resonant Raman process. In this work, we present an analytical model that reveals the physics behind the strikingly different orders of magnitude in enhancement that have been observed, provide a fundamental explanation for the quenching effect observed in fluorescence and resonance Raman but not in normal Raman, establish limits for attainable enhancement, and outline the path to optimization of all three processes.